

# Using the expert model PERPEST to translate measured and predicted pesticide exposure data into ecological risks

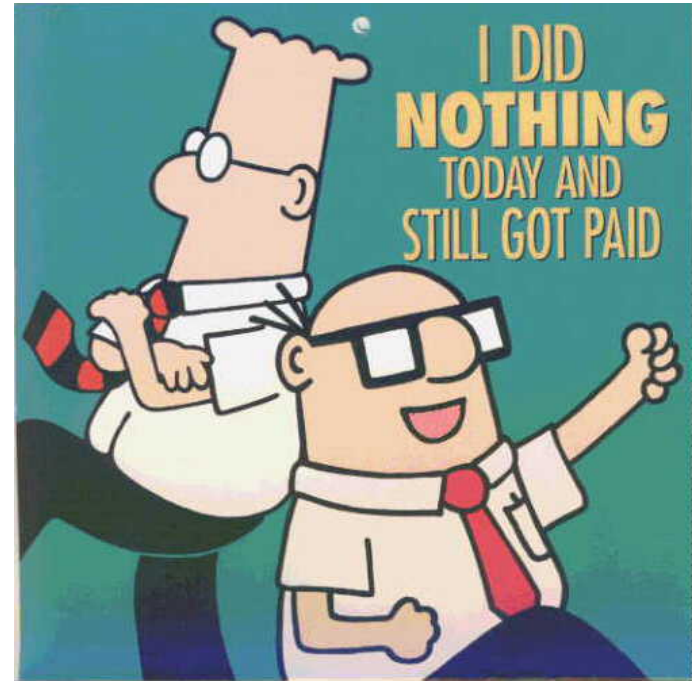
**ECEM/EAML 2004, Bled, Slovenia**

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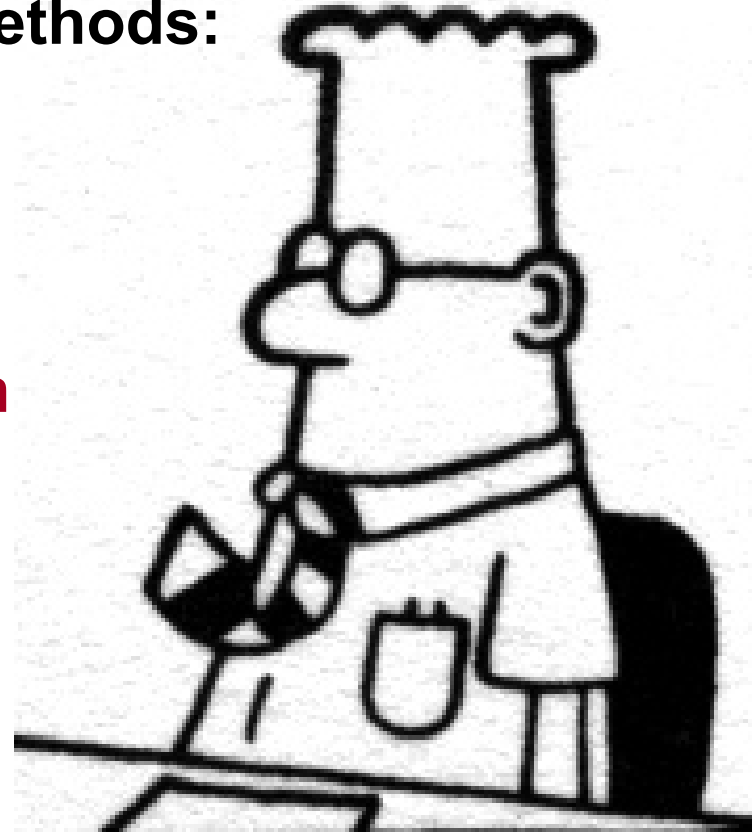
# Why this presentation?

- **To predict the future**
- **Dilbert's philosophy:**  
Many methods to predict the future, but:
- Horoscopes, tea leaves, tarot cards, crystal balls  
→ **nutty methods**
- Putting well-researched facts into sophisticated computer models → **a complete waste of time**



# Why this presentation?

- **Dilbert's method:**
- Use these far more efficient methods:
  1. My awesome powers of **logic**
  2. My crystal-clear **observations**
  3. My almost frightening **intuition**
  4. My total **lack of guilt**



# Case-Based Reasoning

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- Reasoning by **remembering**
- Approach to **problem solving and learning**
- Works **the same as people** use cases to solve problems
- **A methodology**
  - to model human reasoning and thinking
  - for building intelligent computer systems

# Case-Based Reasoning

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- Store previous experience (cases) in **memory**
- To solve **new problems**:
  - **retrieve similar experience** about similar situations from the memory
  - **Reuse and adapt** the experience in the context of the new situation
- Store **new experience** in memory (learning)

# Case-Based Reasoning: PERPEST

## PERPEST

a model to Predict the Ecological Risks of PESTicides

perpest



PERPEST - substance data

Experiment features | Weigh using | Select using | Options

Substance: Atrazine; CAS #1912-24-9

Features:

Feature	Value
Code of substance	1912-24-9
Name of the substance	Atrazine
Type of substance	Herbicide
Mode of action	Photosynthesis inhibitor
Molecule group	Triazin(on)e
LEC50, µg/L	67
dT50, d	77
Henry coefficient, partitioning coeff	1.015E-7
Partitioning coefficient water-organic	70

Number of cases: 64

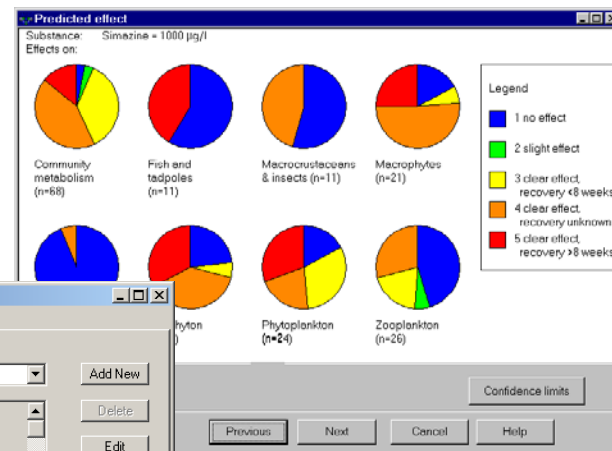
Concentration (µg/l): 500 = 7.463 toxic units

Exposure: multiple/constant

Type of experiment: stagnant

Number of effect classes: 5

Buttons: Previous, Next, Cancel, Help, Reset

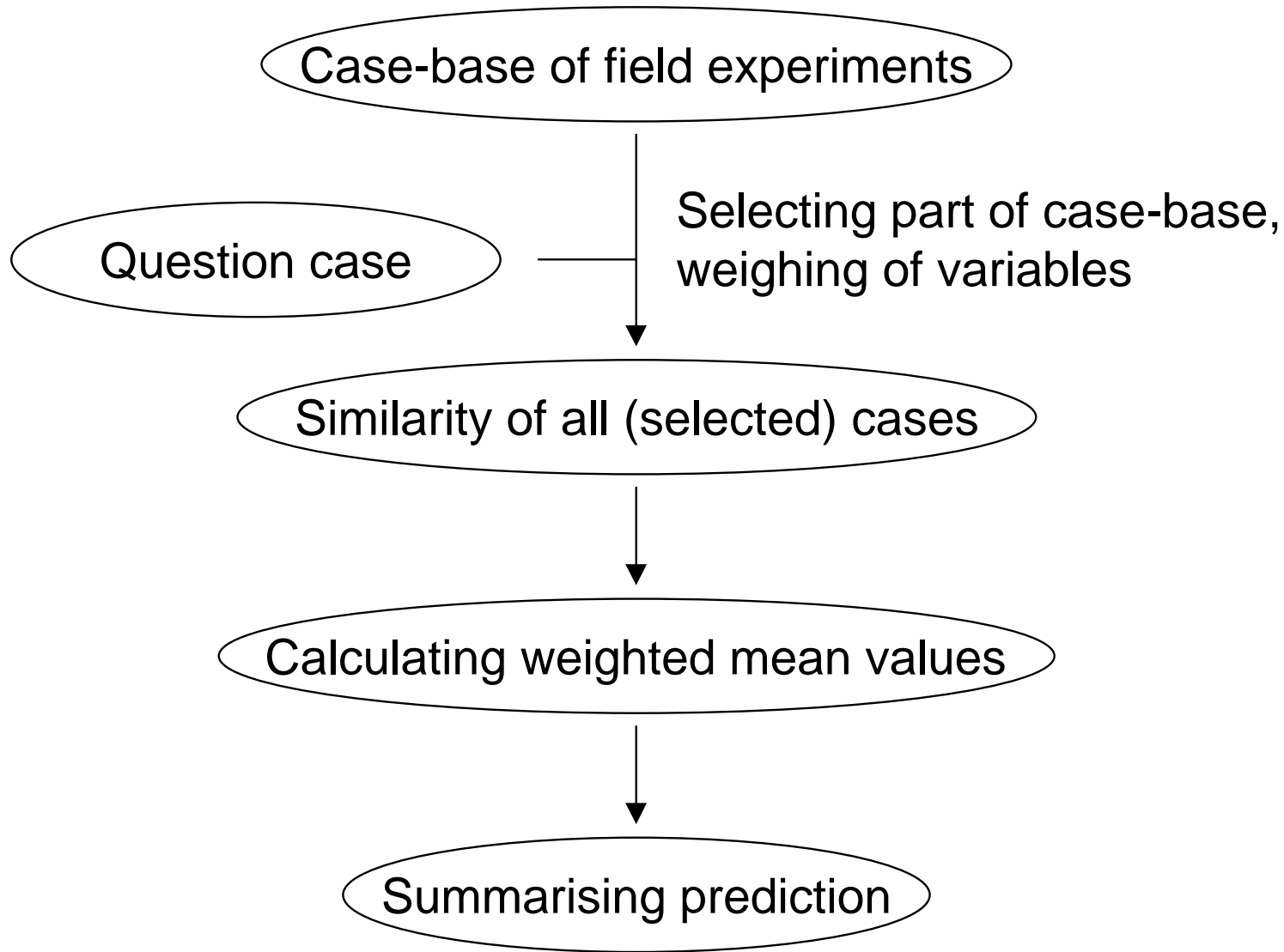


# Case-Based Reasoning: PERPEST

- **Aim:** Predict effects of pesticides on freshwater ecosystems
- **Case-Base:** Results from microcosm and mesocosm experiments



# Case-Based Reasoning: PERPEST



# Case-Based Reasoning: PERPEST

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## Case base:

- **Field Experiments** evaluating effects of insecticides and herbicides using microcosms or mesocosms
- Passed several **quality criteria** (e.g. description of set-up is adequate, endpoints are sensitive)
- **90 experiments** evaluated (1980-2002) → **421 records** (substance \* concentration)  
208 herbicide records, 213 insecticide records
- Effects evaluated on **8 groups of endpoints**

# Case-Based Reasoning: PERPEST

- **Case-Base:** Results from microcosm and mesocosm experiments

C A S E  1	<b>Problem</b>	
	Problem: effect of Atrazine	
	Concentration: 500 µg/L	
	Reference: DeNoyelles et al., 82, 89, 94	
	Exposure: multiple/constant	
	Type of ecosystem: stagnant/recirculating	
	<b>Solution (effects observed)</b>	
	Grouped endpoint	Effect class
	Community metabolism	3
	Phytoplankton	5
	Periphyton	0
	Macrophytes	5
	Zooplankton	4
	Macrocrustaceans & Insects	4
	Other macro-invertebrates	1
	Vertebrates	5



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# Case-Based Reasoning: PERPEST

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- **Effect classes:**
  0. Endpoint not evaluated in the study.
  1. No effects demonstrated
  2. Slight effects.
  3. Clear short-term effects, lasting  $< 8$  weeks
  4. Clear effects, recovery not studied
  5. Clear long-term effects, lasting  $> 8$  weeks
- **Resulting database:  $421 * 8 = 3368$  entries  
(1424 non-zeros)**

# Case-Based Reasoning: PERPEST

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## Grouped endpoints:

### Herbicides

- Community metabolism
- Phytoplankton
- Periphyton
- Macrophytes
- Zooplankton
- Macrocrustaceans & Insects
- Other macro-invertebrates
- Vertebrates

### Insecticides

- Community metabolism
- Algae and macrophytes
- Microcrustacea
- Rotifers
- Macrocrustacea
- Insects
- Other macro-invertebrates
- Vertebrates

# Case-Based Reasoning: PERPEST

## Data selection/weighting database

For every chemical or experiment:

- Concentration of every case is **standardised on the EC50** of the most standard test species (concentration/EC50) to make concentrations between chemicals comparable
- **Type exp.:** acute/chronic, stagnant/flow-through  
**Fate:** DT50, Henry coefficient, Kom  
**Molec. type:** Insecticide/herbicide, Molecule group, Toxicological mode of action

# Case-Based Reasoning: PERPEST

- **Input**

PERPEST - substance data

Experiment features | Weight/Select using | Options

Substance: Chlorpyrifos; CAS =2921-88-2 Add New

Features:

Feature	Value
Code of substance	2921-88-2
Name of the substance	Chlorpyrifos
Type of substance	Insecticide
Mode of action	Acetylcholinesterase inhibitor
Molecule group	Organophosphate
EC50 (µg/L)	0.19
DT50 (days)	1
Henry coefficient (Pa m <sup>3</sup> /mol)	0.676
K <sub>ow</sub> (L/kg)	3469

Delete  
Edit

Number of cases: 40

Concentration (µg/l): 10 = 52.63 toxic units

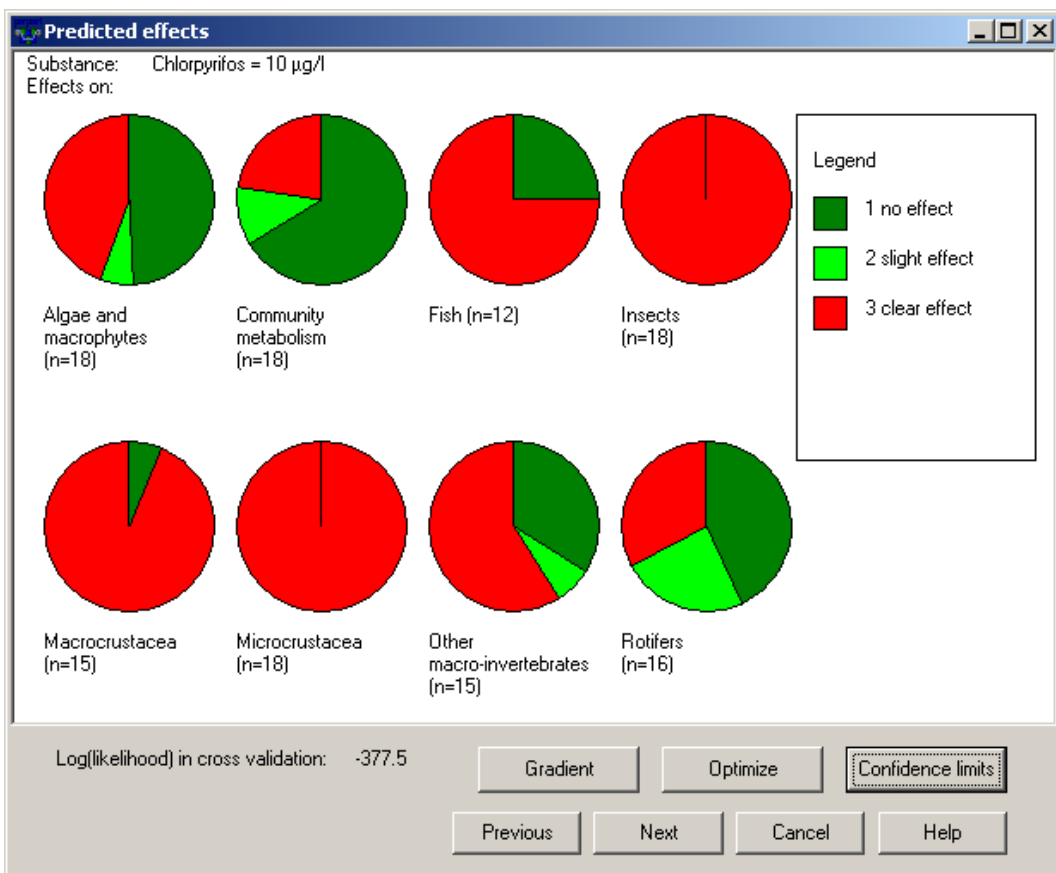
Number of effect classes: 3  
3  
5 Reset

Load Previous Next Cancel Help

# Case-Based Reasoning: PERPEST

- Effects of chlorpyrifos (10 µg/L), **weight parameters optimised**

**C.L.** using bootstrapping:



Variable	Prediction	5% CL	95% CL	N
(Is) Insects = 1	0.00	0.00	0.00	18
(Is) Insects = 2	0.00	0.00	0.00	18
(Is) Insects = 3	1.00	1.00	1.00	18
(Is) Macrocrustacea = 1	0.06	0.00	0.21	15
(Is) Macrocrustacea = 2	0.00	0.00	0.00	15
(Is) Macrocrustacea = 3	0.94	0.79	1.00	15
(Is) Rotifers = 1	0.43	0.21	0.68	16
(Is) Rotifers = 2	0.24	0.06	0.46	16
(Is) Rotifers = 3	0.33	0.10	0.57	16

# Case-Based Reasoning: PERPEST

- Most **similar** cases

Browse cases analogous with Chlorpyrifos = 10 µg/l

Order of this record: 2 [K] [ < ] [ > ] [ | ] Dissimilarity: 7.327E-6

Variable	Value	Effect on	Value
Code of substance	2921-88-2	Algae and macrophytes	1
Name of the substance	Chlorpyrifos	Community metabolism	-
Type of substance	Insecticide	Fish	-
Mode of action	Acetylcholinesterase int	Insects	-
Molecule group	Organophosphate	Macrocrustacea	-
Concentration of substance, ug/l	10	Microcrustacea	3
Concentration as toxic unit	52.632	Other macro-invertebrates	-
Exposure	single/pulse	Rotifers	-
Hydrology during experiment	Stagnant/Recirculating		

Reference: Hughes et al. 1980

Previous Finish Cancel Help

Browse cases analogous with Chlorpyrifos = 10 µg/l

Order of this record: 3 [K] [ < ] [ > ] [ | ] Dissimilarity: 0.4232

Variable	Value	Effect on	Value
Code of substance	2921-88-2	Algae and macrophytes	-
Name of the substance	Chlorpyrifos	Community metabolism	1
Type of substance	Insecticide	Fish	3
Mode of action	Acetylcholinesterase int	Insects	3
Molecule group	Organophosphate	Macrocrustacea	-
Concentration of substance, ug/l	6.3	Microcrustacea	3
Concentration as toxic unit	33.158	Other macro-invertebrates	3
Exposure	single/pulse	Rotifers	3
Hydrology during experiment	Stagnant/Recirculating		

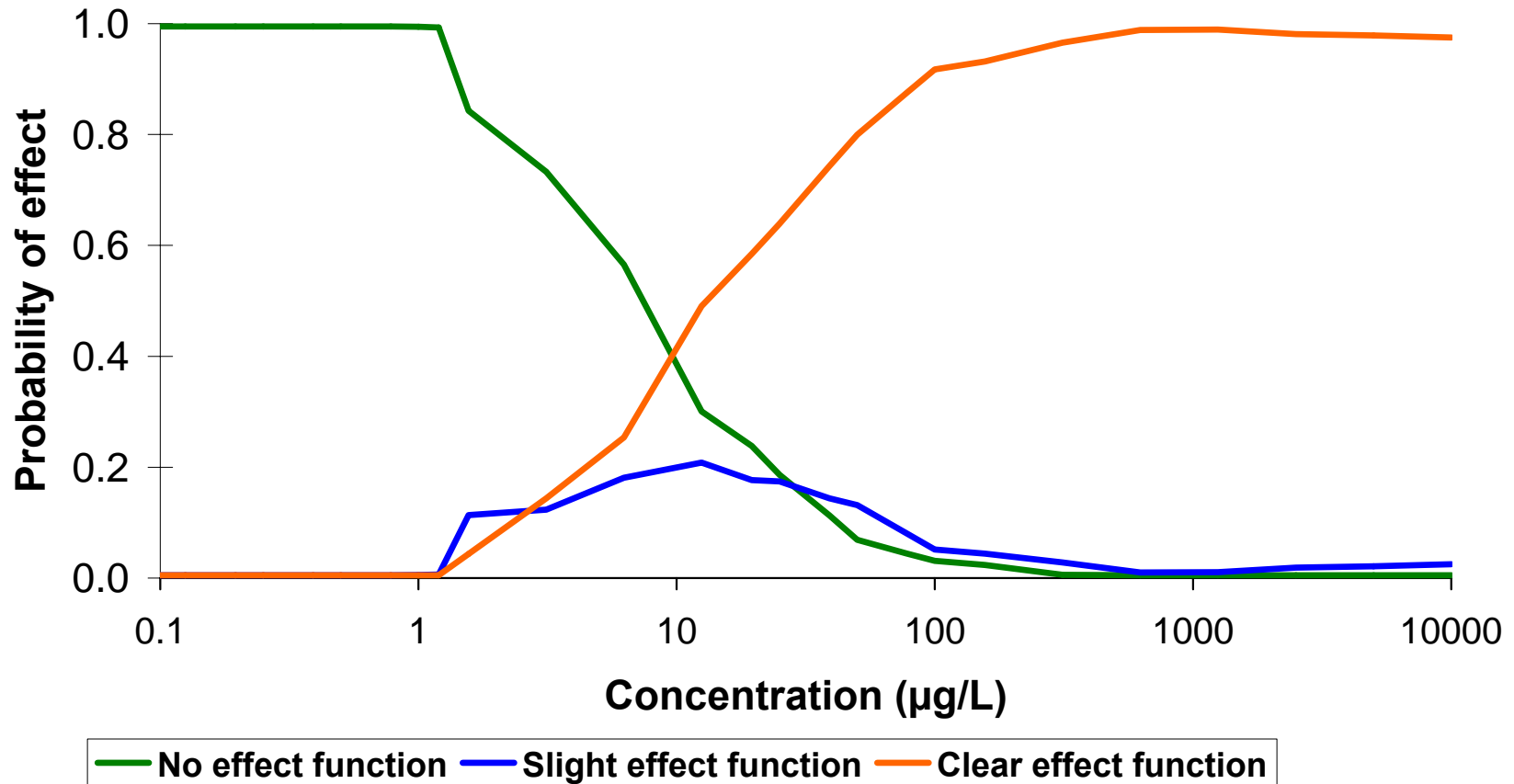
Reference: Siefert et al. 1989

Previous Finish Cancel Help

# Case-Based Reasoning: PERPEST

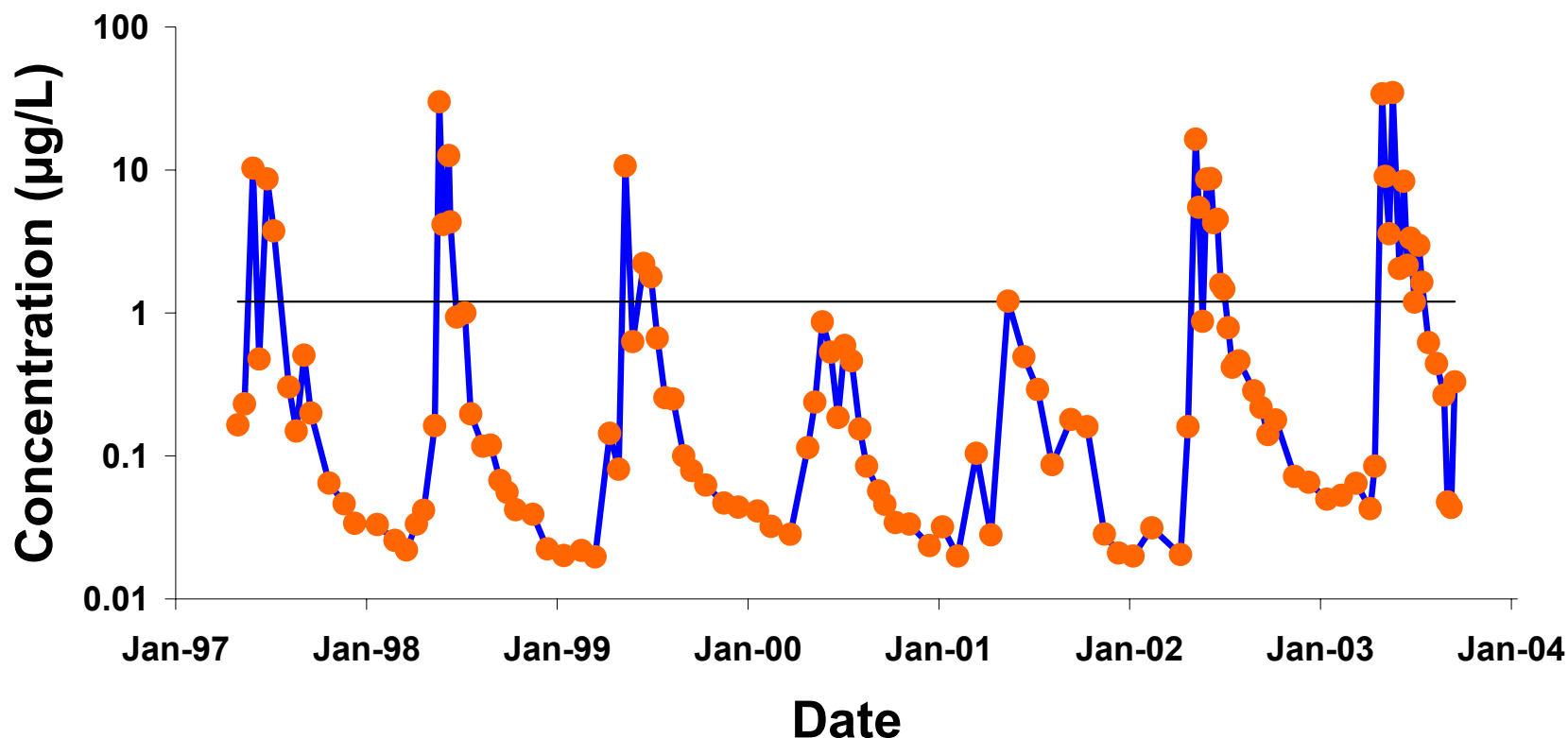
- Predict effects over a **concentration range**

Effects of atrazine on functional endpoints



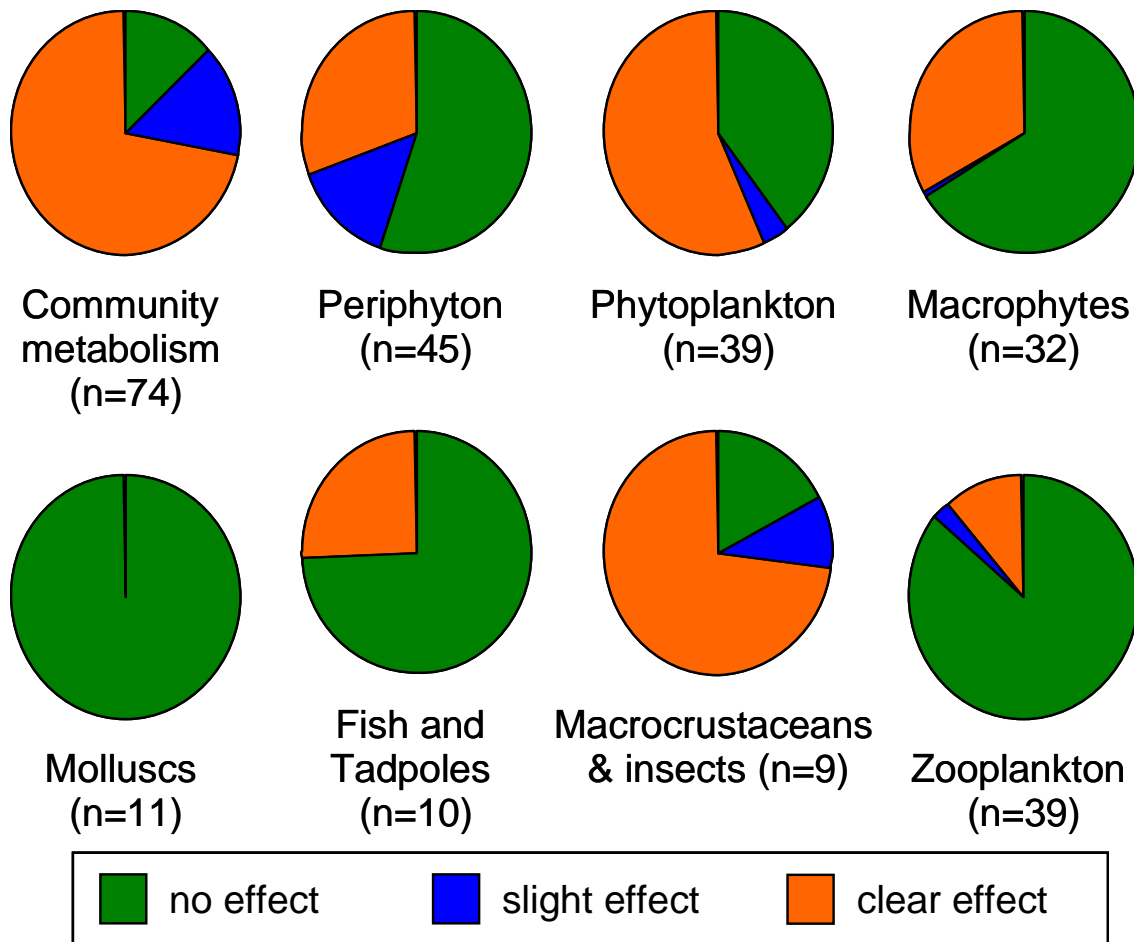
# PERPEST: combining with measured data

- Maple Creek (Nebraska)
- 30-04-97 to 16-09-03: **124 values**
- Max = **34.8  $\mu\text{g/L}$** ; geomean = **0.27  $\mu\text{g/L}$**



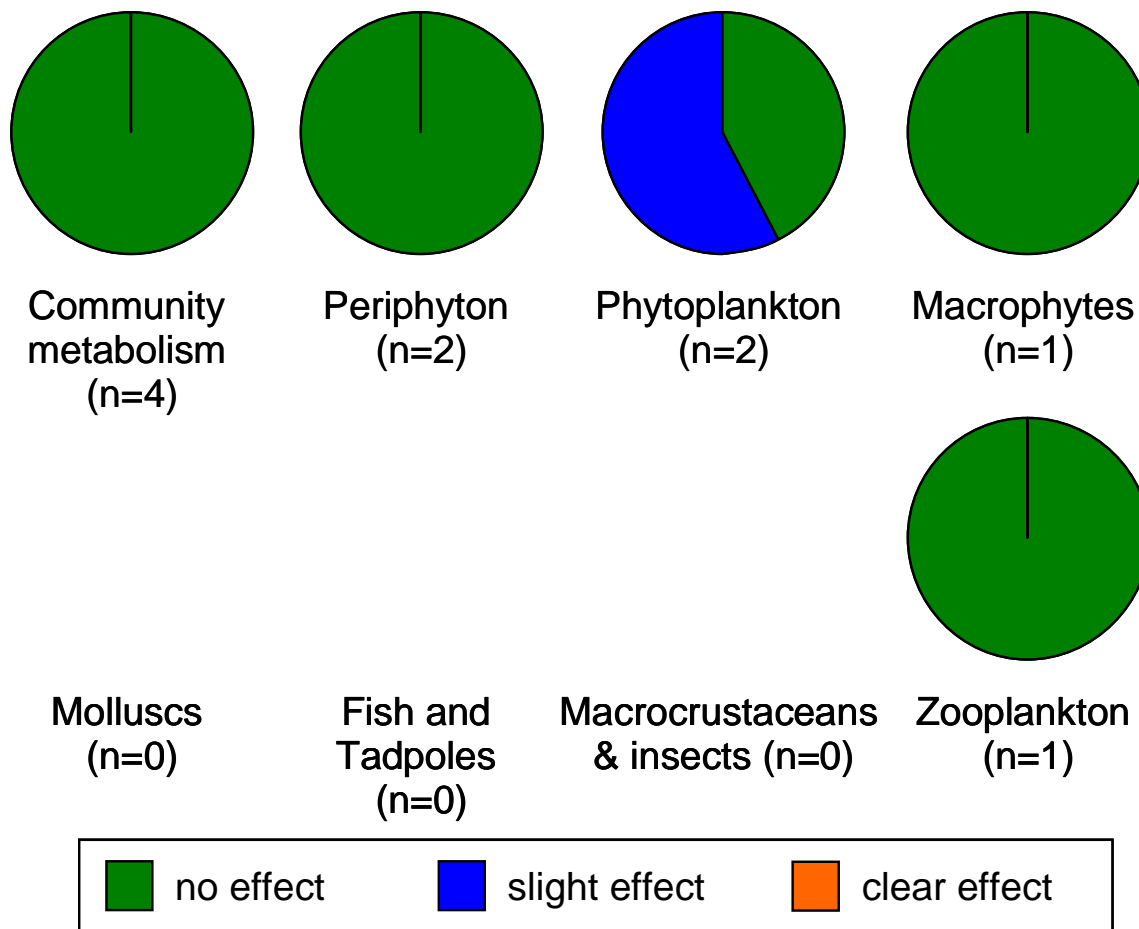
# PERPEST: combining with measured data

- Effects of maximum concentration: = 34.8 µg/L



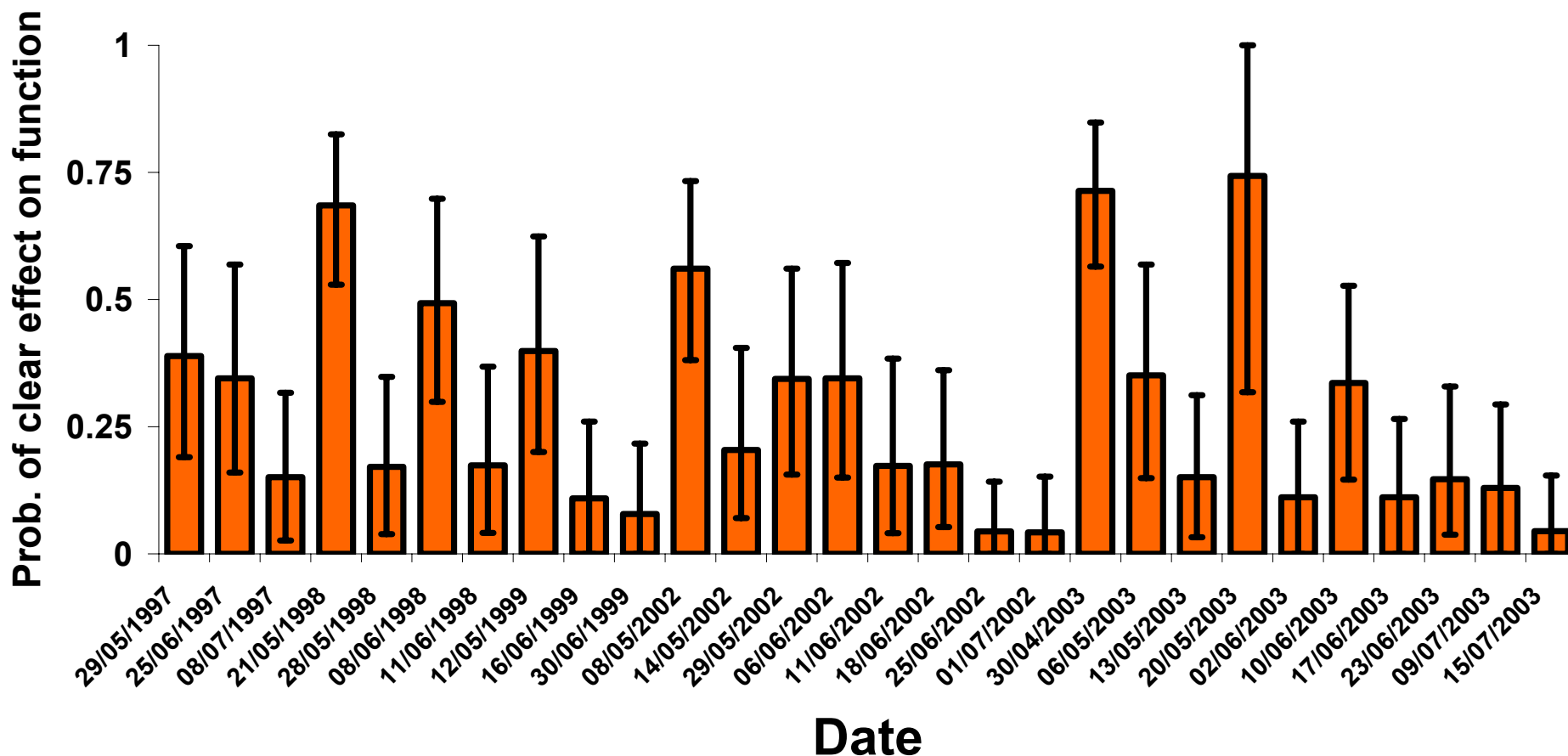
# PERPEST: combining with measured data

- Effects of medium concentration: = **0.27 µg/L**



# PERPEST: combining with measured data

- **Probability** of measured concentrations leading to clear effects on **functional endpoints**

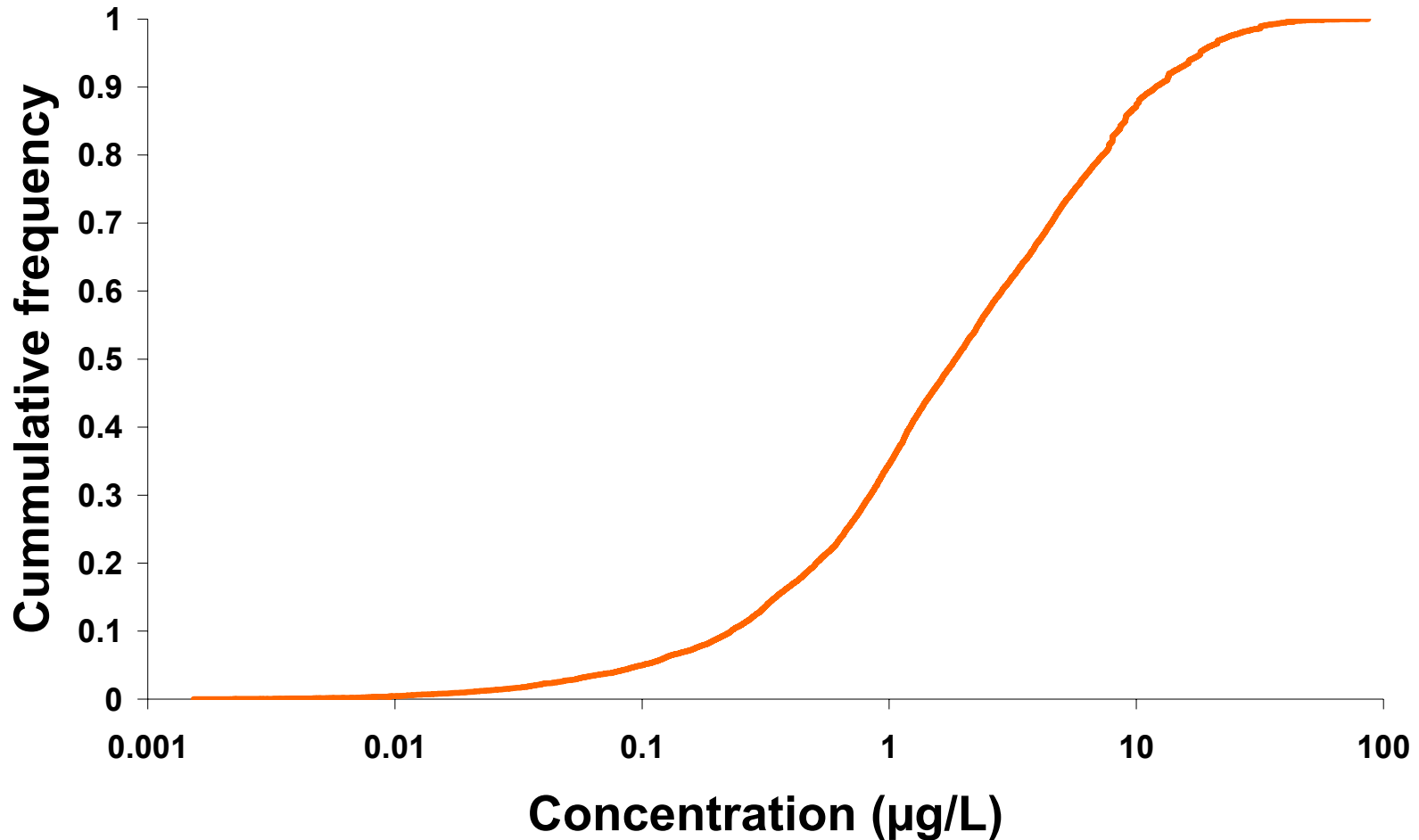


# PERPEST: combining with measured data

- **Functional: in 43% of the cases: chance > 25% on a clear effect**
- **Functional: in 14% of the cases: chance > 50% on a clear effect**
- **Structural: 43 and 11%, respectively**
- **(1) If the structure and functioning of the model-ecosystems as well as the (2) exposure regime, used in the experiments incorporated in PERPEST are representative for Maple Creek:**
  - **it is very likely that atrazine contamination affected the aquatic community during the last 7 years, in particular in the year 2003.**

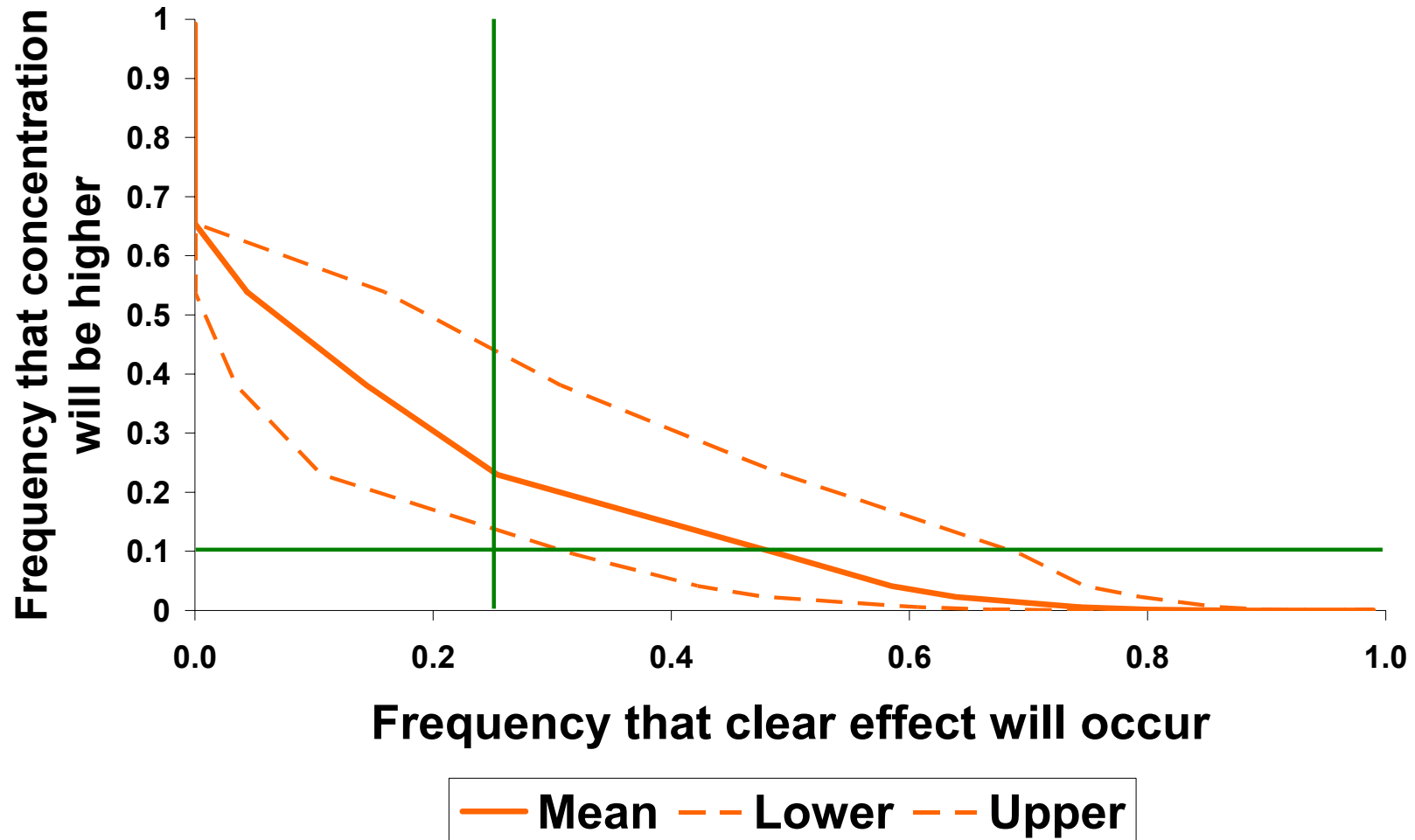
# PERPEST: combining with modelled data

- **Cumulative Distribution Function modelled conc.:**



# PERPEST: combining with modelled data

- **Joint Probability Curve: Clear effects on function**

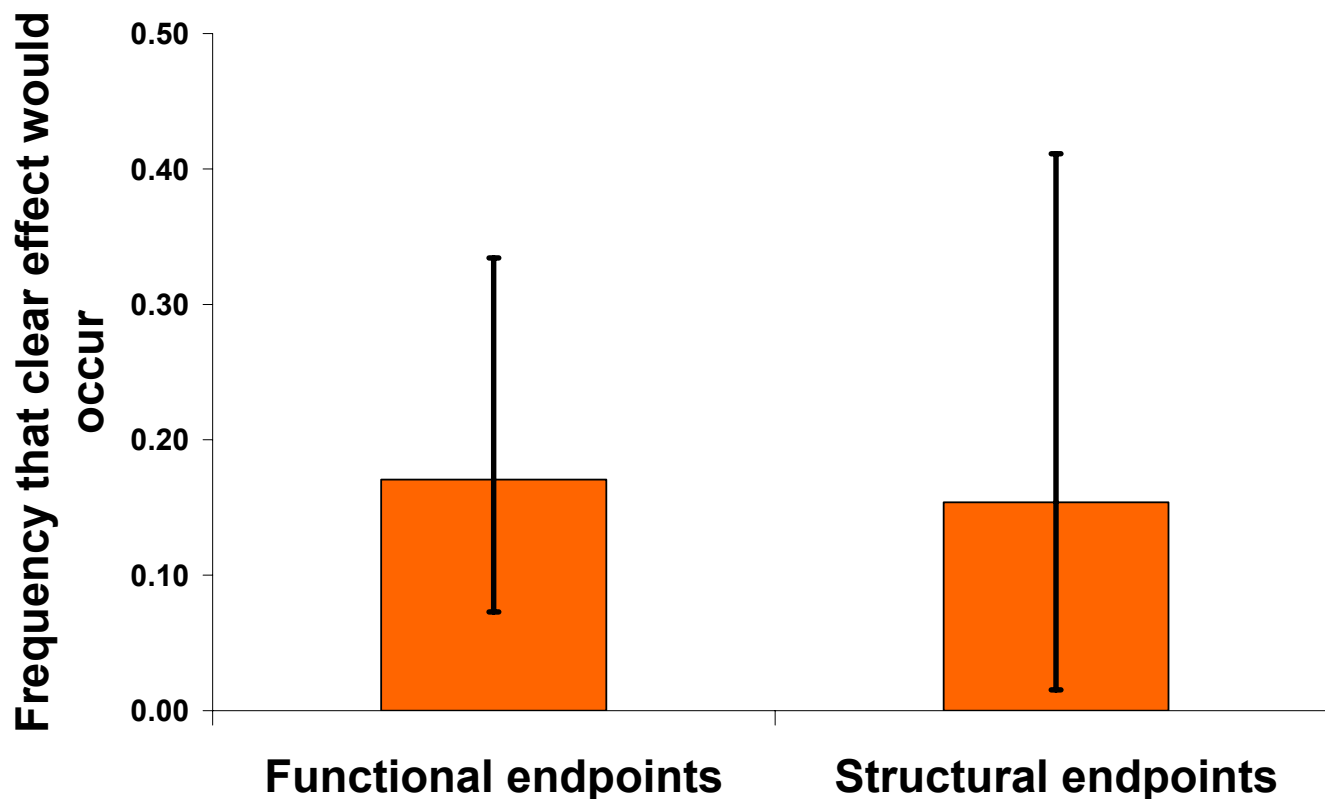


## PERPEST: combining with modelled data

- The **90% exposure concentration** (= 0.1 frequency on y-axis) is estimated to result in clear effects on community metabolism with a frequency of **49%** (95% confidence interval 31 – 69%),
- A **25% frequency of clear effects** on community metabolism occurs for **77%** (95% confidence interval 56-86%) of the exposure distribution,
- **assuming** that
  1. the exposure model is correct and
  2. that mesocosm studies directly represent effects in the field.

# PERPEST: combining with modelled data

- Both axes of JPC are proportions of application events, so can be combined to estimate the overall frequency that clear effects would result → area under the curves



# PERPEST: discussion

- A **key advantage** of PERPEST over single species tests and safety factors is that it **removes the uncertainty of extrapolating** to the ecosystem level
- PERPEST makes some **assumptions**, however:
  1. The cases are **representative** for the question case with respect to ecosystem structure and functioning and exposure regime
  2. The calculations of dissimilarity and transformation, standardisation and weighing of variables are **adequate** for making predictions
  3. The number of cases is **sufficient** for making a prediction
  4. **????? Please add !!!!!**

# PERPEST: discussion

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- PERPEST **might underestimate effects** for measured concentrations → water samples not been taken at highest concentrations
- **Shortcoming of chemical monitoring** in general, not of PERPEST
- PERPEST can evaluate monitoring activities in the light of the **Water Framework Directive**
- **Overall risk of pesticides with similar mode of action** can be assessed by adding chemicals up as toxic units
- Dissimilar mode of actions can be combined using response addition to an **overall risk of all pesticides measured**

# PERPEST: discussion

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- Obvious **drawbacks**:
  1. often only very **few** really comparable cases are available; and,
  2. specific cases are often too easily **generalised**
- Seek the **best of both worlds** by:
  1. using **CBR** as a mimic of the experts' approach and
  2. fine-tuning the results with **simple ecological models**
- Empirical models + ecological models = **model-based adaptation**

# PERPEST: overview

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- **Semi-field database** is published (Brock et al., 2000a,b) and updated last year (2003)
- **Scientific paper** published in ET&C (2002), **Manual published** as Alterra report (2003), **Scientific paper for this conference** (2004)
- **Model, paper and manual are available** via [www.perpest.alterra.nl](http://www.perpest.alterra.nl)
- Data on **fungicides** will be added next year

# Why this presentation?

Dilbert's method:

1. My awesome powers of logic
  - Events in the past are predictive for the future
2. My crystal-clear observations
  - I did a good job reviewing all these microcosm and mesocosm experiments
3. My almost frightening intuition
  - Other traits than concentrations alone also matter (like type exp., fate and molecule type)
4. My total lack of guilt
  - Detail doesn't matter (i.e. ignore assumptions)

